**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

| | |
|---|---|
| Applicant(s): McCollor, et al. | |
| Application No.: 10/666,528 | Group Art Unit: 1793 |
| Filed: September 19, 2003 | Examiner: LANGEL, WAYNE A. |
| Title: METHOD AND APPARATUS FOR CAPTURING GAS PHASE POLLUTANTS SUCH AS SULFUR TRIOXIDE | Attorney Docket No.: EER.P0014 |

## SECTION 1.132 DECLARATION OF DONALD MCCOLLOR

Commissioner for Patents
PO Box 1450
Alexandria, VA 22313-1450

I, Donald McCollor, hereby declare the following:

1. I am a co-inventor of patent application Serial Number 10/666,528 filed on 9/19/2003, referenced above.

2. I understand that the Examiner has rejected the claims under § 112, first paragraph, as failing to comply with the enablement requirement. I understand that the Examiner has stated that the applicants have not explained where the specification provides enablement for properly programming the CHEMKIN and FLUENT computer models to perform the disclosed and claimed functions.

3. CHEMKIN is an off-the-shelf software tool for solving complex chemical kinetics problems. CHEMKIN is a set of flexible tools for incorporating complex chemical kinetics into simulations of reacting flow. Using CHEMKIN, users are able to investigate thousands of reaction combinations to develop a comprehensive understanding of a particular process, which might involve multiple chemical species, concentration ranges, and gas temperatures. One skilled in the art understands what CHEMKIN can do, as well as how to properly configure and program

CHEMKIN to perform various functions. Further, the maker of CHEMKIN provides detailed instructions and manuals relating to the use of CHEMKIN. To provide further information about CHEMKIN, a CHEMKIN brochure is attached to this Declaration.

4. FLUENT is off-the-shelf computational fluid dynamics (CFD) flow modeling software. FLUENT can be used to calculate gas velocity and temperature in a combustion system. One skilled in the art understands what FLUENT can do, as well as how to properly configure and program FLUENT to perform various functions. Further, the maker of FLUENT provides detailed instructions and manuals relating to the use of FLUENT. To provide further information about FLUENT, a FLUENT brochure is attached to this Declaration.

5. I hereby declare that all statements made herein of my own knowledge are true, and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code, and that such willful false statements may jeopardize the validity of the application, any patent issuing thereon, or any patent to which this verified statement is directed.

08/27/08
Date

Donald P. McCollor
Donald McCollor

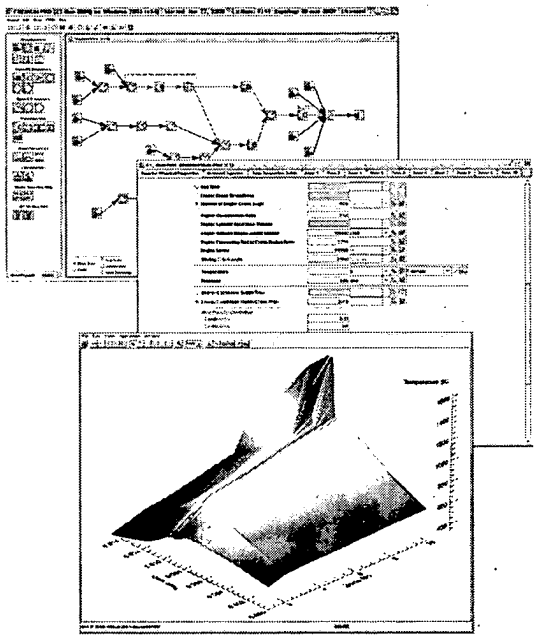
reaction
DESIGN

# CHEMKIN

LEADING SOLUTIONS FOR THE RAPID SIMULATION OF COMPLEX CHEMISTRY

# Chemistry Simulation Enables Clean Technology Design

Understanding and predicting chemistry effects is essential in developing Clean Technology solutions in transportation, energy and materials processing applications. As gas turbine, boiler and piston engine designers strive to meet low-emissions regulations with ever widening fuel flexibility, they must also maintain, or even improve, their system's performance. Relying on engine testing for accurate performance validation is prohibitive, given today's fuel diversity, complex engine designs and shortening design cycles. Effective simulation of the underlying detailed combustion chemistry is required for cost-effective design of systems with reduced pollutant emissions.



## CHEMKIN® — the de facto standard simulation tool for solving complex chemical design problems

At its most fundamental level, CHEMKIN software enables the simulation of complex chemical reactions. With the advanced capabilities now available, sophisticated Design-of-Simulations (DoS) can be created to parametrically explore potential design solutions well before costly hardware is built.

CHEMKIN evolved from its origin as a Sandia National Laboratory combustion code (Chemkin II) into today's commercial-quality software suite with a user-friendly interface, best-in-class simulation speed, and unparalleled accuracy. No other chemistry simulation product is more widely validated or cited in technical peer-reviewed journals.

Reaction Design offers multiple CHEMKIN products to satisfy unique requirements. CHEMKIN-PRO™ is specifically designed for large chemical simulation applications requiring complex mechanisms. CHEMKIN-PRO's advanced solvers and full feature set support the quick and accurate development of models for specific applications. CHEMKIN 4 provides industry-leading simulation technology for the simulation of less complex systems at an affordable price. CHEMKIN-CFD™ extends the power of CHEMKIN into Computational Fluid Dynamics (CFD) and enables the introduction of more accurate chemistry into reacting, fluid flow simulations.

| FEATURE COMPARISON | CHEMKIN-PRO | CHEMKIN 4 |
|---|---|---|
| Combustion Reactors | • | • |
| Surface Chemistry | • | • |
| Parameter Study | • | • |
| Reactor Networks | Enhanced | Basic |
| Solver Speed | Enhanced | Basic |
| Reaction Path Analyzer | • | |
| Multi-Zone Engine Model | • | |
| Particle Tracking | • | |
| Uncertainty Analysis | • | |
| 64-bit Support | • | |

## CHEMKIN-PRO — fast, accurate chemistry for power users

Incorporating advanced functionality and the latest analytical algorithms and methods, CHEMKIN-PRO delivers the ultimate in speed, accuracy and solution robustness.

### *Accurate solutions, in a fraction of the time*

For complex models with large mechanisms, core solver enhancements incorporated into CHEMKIN-PRO cut simulation times from days to hours, or hours to minutes. CHEMKIN-PRO can be over 20 times faster than previous versions of CHEMKIN in demanding applications.

### *A whole new view*

To help you gain key insights into kinetics dependencies, CHEMKIN-PRO includes the Reaction Path Analyzer. Employing an interactive, visual display, the Reaction Path Analyzer provides a clear view of dominant reaction paths that facilitate mechanism development and reduction.

### *Use complex flow-field representations to enable more accuracy*

Enabling the most efficient prediction of emissions with detailed chemistry, Equivalent Reactor Networks allow you to link mixed-type reactors representing real world designs.

### *Understand and predict soot and particle formation*

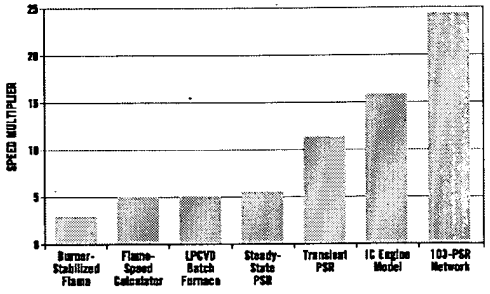
The innovative Particle Tracking feature of CHEMKIN-PRO follows particle inception, growth and oxidation. You can apply number and size statistics to predict soot emissions or optimize particle production.

### *Explore how input uncertainties affect simulation results*

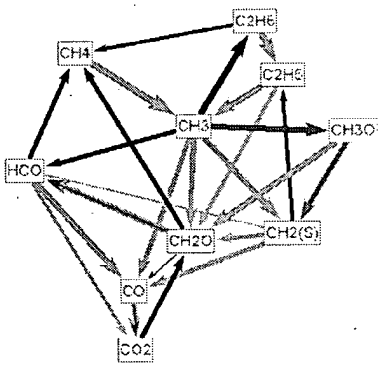
Enhance the robustness of simulation results with the ability to calculate error bars based on user-defined input accuracy ranges.

### *Multi-Zone Engine Model for piston engines*

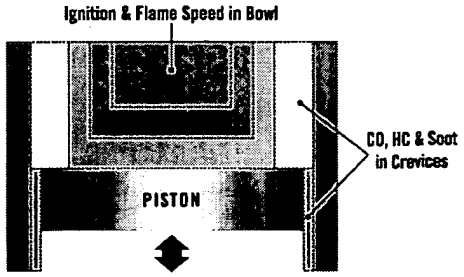
CHEMKIN-PRO's Multi-Zone Engine Model simplifies and optimizes the analysis of key combustion effects including ignition, flame speed, plus CO, HC and Soot emissions.




*Simulation Speed-Up of CHEMKIN-PRO vs. CHEMKIN 4.1*




*Visualize reactions with the Reaction Path Analyzer*




*Multi-Zone Engine Model*

# CHEMKIN

## CHEMKIN 4 — Industry-leading technology in an affordable, flexible and easy to use solution

For developers who do not require the speed or advanced features offered in CHEMKIN-PRO, Reaction Design offers CHEMKIN 4 as an economical alternative. Up to 5x faster than freeware and academic codes, CHEMKIN 4 is a robust and mature chemistry simulation tool that has been widely used for an impressive range of applications. CHEMKIN 4 is a cost effective solution for simulation projects employing small or reduced mechanisms and/or comprise less complex reactions.

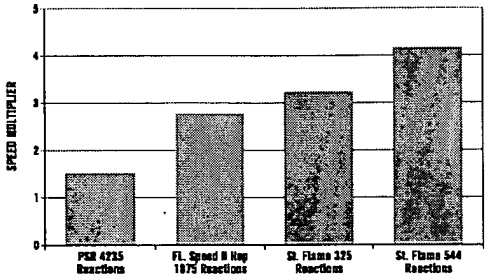
## CHEMKIN-CFD — Detailed kinetics modeling meets CFD

CFD software has become a standard design tool for combustor and engine designers. Most CFD cases are run with simplified, or global mechanisms, because computation time prohibits use of more detailed chemistry. However, emission predictions, ignition and stability issues require a much more detailed accounting of chemistry effects to ensure useful analysis. To solve complex, chemical kinetics problems faster and more accurately, Reaction Design enables detailed kinetics modeling through its CHEMKIN-CFD software package. CHEMKIN-CFD couples with, and extends the capabilities of, leading CFD software and engine modeling software from CD-Adapco Group, Fluent (ANSYS, Inc), Gamma Technologies, Ricardo plc, and Los Alamos National Laboratory (KIVA).

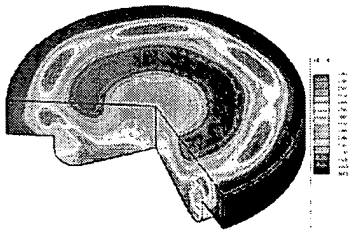
## About Reaction Design

Reaction Design empowers transportation manufacturers and energy companies to achieve their Clean Technology goals with comprehensive and easy-to-use software simulation tools, chemical models and expert consulting services. Reaction Design is the exclusive developer and distributor of CHEMKIN — the de facto standard for modeling and simulating gas-phase and surface chemistry. Reaction Design also provides the CHEMKIN-CFD software package, extending the capabilities of leading computational fluid dynamics (CFD) programs. Reaction Design's world-class engineers, chemists and programmers have expertise that spans multi-scale engineering from the molecule to the plant.

**To learn more about how CHEMKIN products can help you solve your most complex chemical design problems, email info@reactiondesign.com or visit www.reactiondesign.com**




*Simulation Speed-Up of CHEMKIN 4.1 vs. Chemkin II*



*Combustion in this heavy-duty diesel was simulated with a 26-step mechanism using Star-CD/CHEMKIN-CFD*
*(Courtesy of the CD Adapco Group)*


**Reaction Design**
6440 Lusk Boulevard, Suite D-205
San Diego, CA 92121

*web:*
www.reactiondesign.com

*telephone:*
(+1) 858-550-1920

*fax:*
(+1) 858-550-1925

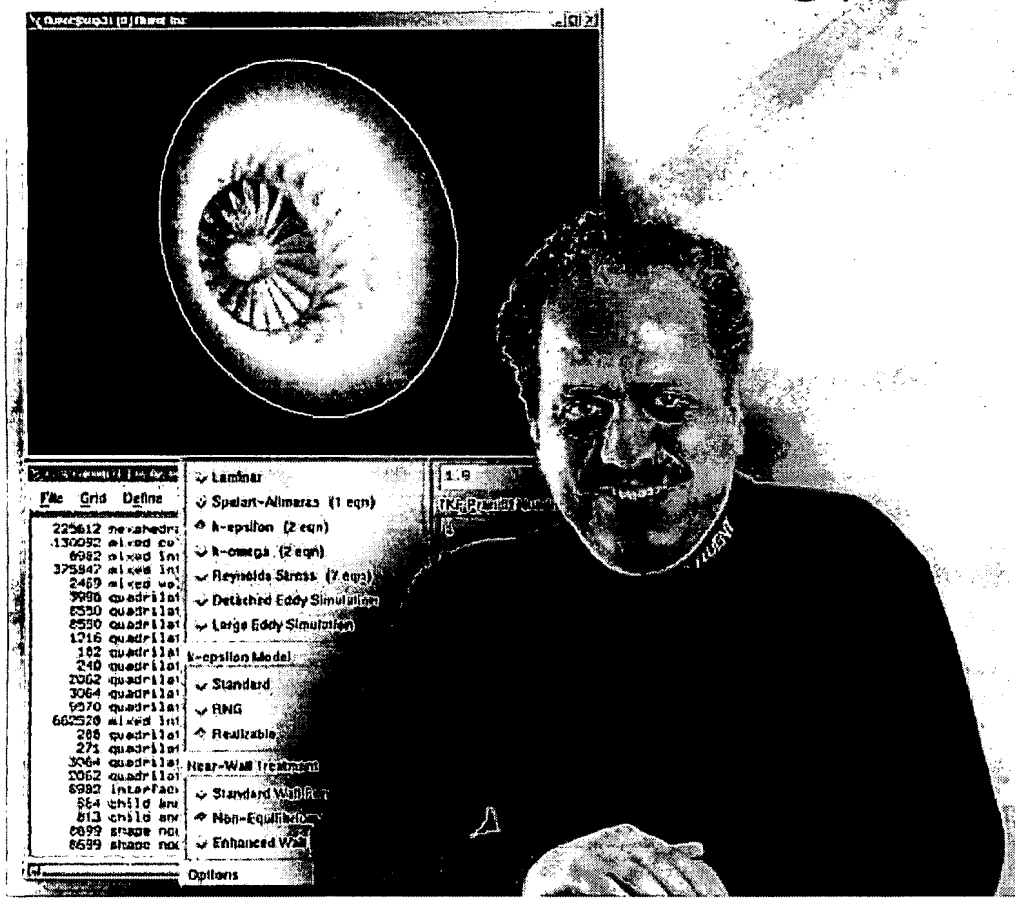
*sales information:*
sales@reactiondesign.com

*technical support:*
support@reactiondesign.com




reaction
DESIGN

# FLUENT
# Flow Modeling Software

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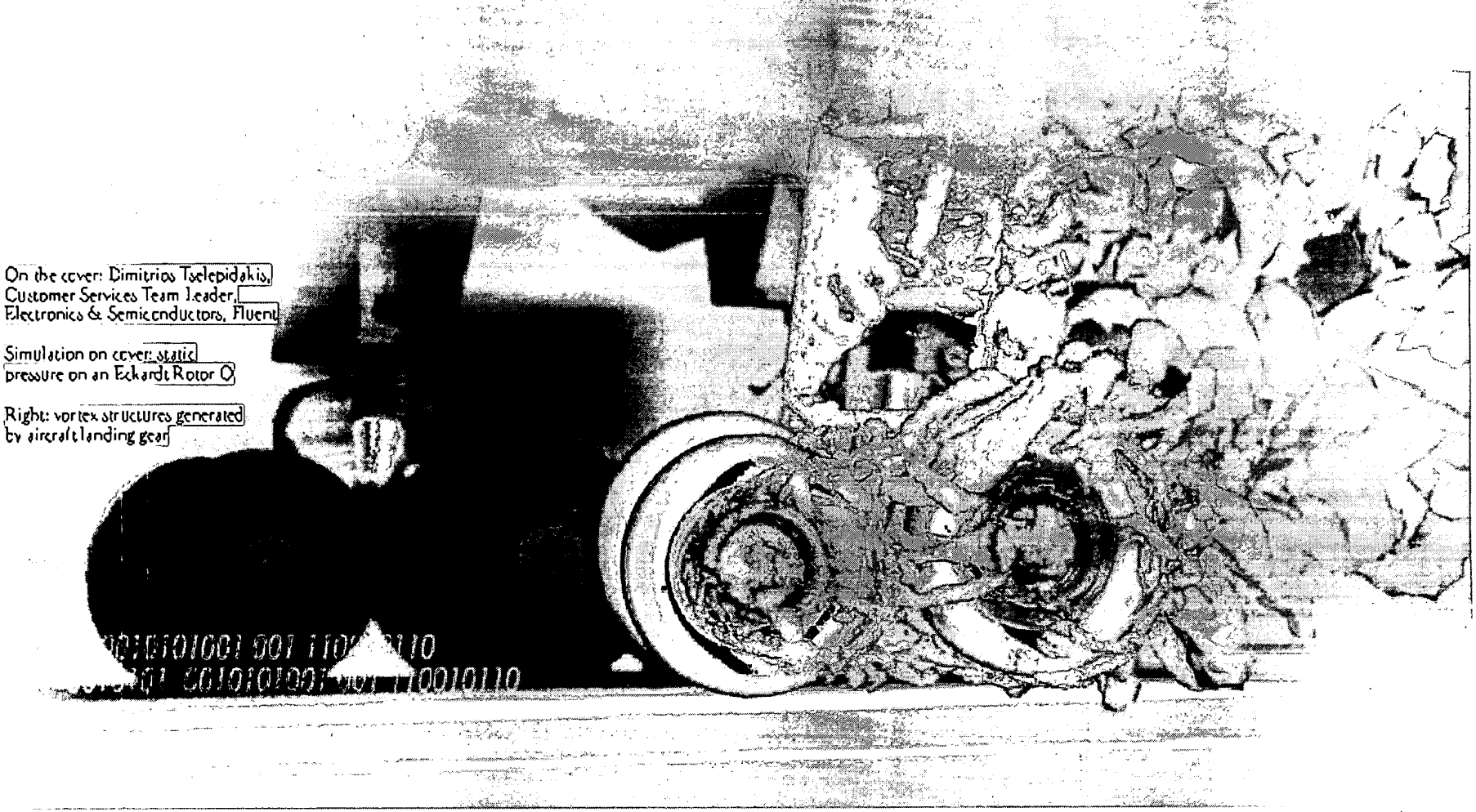
FLUENT
The Right Answer in CFD

FLUENT. For over twenty years the name has been synonymous with the world's leading commercial software for solving fluid flow problems. Based on a numerical technique called computational fluid dynamics, or CFD, FLUENT has a proven track record for delivering fast, accurate, and meaningful solutions to engineers in dozens of industries worldwide.



On the cover: Dimitrios Tselepidakis, Customer Services Team Leader, Electronics & Semiconductors, Fluent

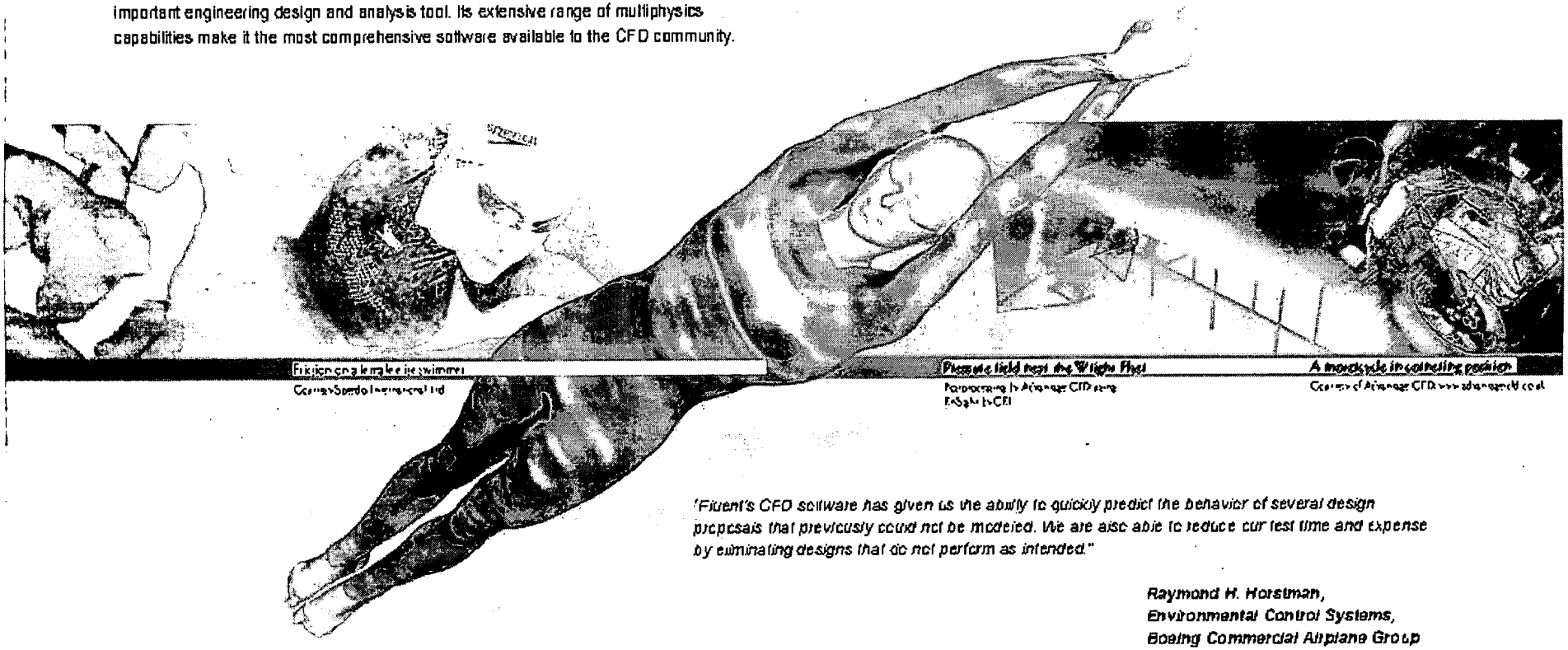
Simulation on cover: static pressure on an Eckardt Rotor O

Right: vortex structures generated by aircraft landing gear

# The Right Answer in CFD

When people think of CFD, the name FLUENT comes to mind. The broad physical modeling capabilities of FLUENT have been applied to industrial applications ranging from air flow over an aircraft wing to combustion in a furnace, from bubble columns to glass production, from blood flow to semiconductor manufacturing, from clean room design to wastewater treatment plants. The ability of the software to model in-cylinder engines, aeroacoustics, turbomachinery, and multiphase systems has served to broaden its reach. Today, thousands of companies throughout the world benefit from this important engineering design and analysis tool. Its extensive range of multiphysics capabilities make it the most comprehensive software available to the CFD community.

With its long-standing reputation of being user-friendly and robust, FLUENT makes it easy for new users to come up to productive speed. Most importantly, technical support is top-notch, from the initial training to the ongoing relationship that develops between customers and Fluent staff. Throughout the years, these important components—comprehensive models, usability, and personalized technical support—have combined to make FLUENT the CFD software of choice across a broad spectrum of industries worldwide.



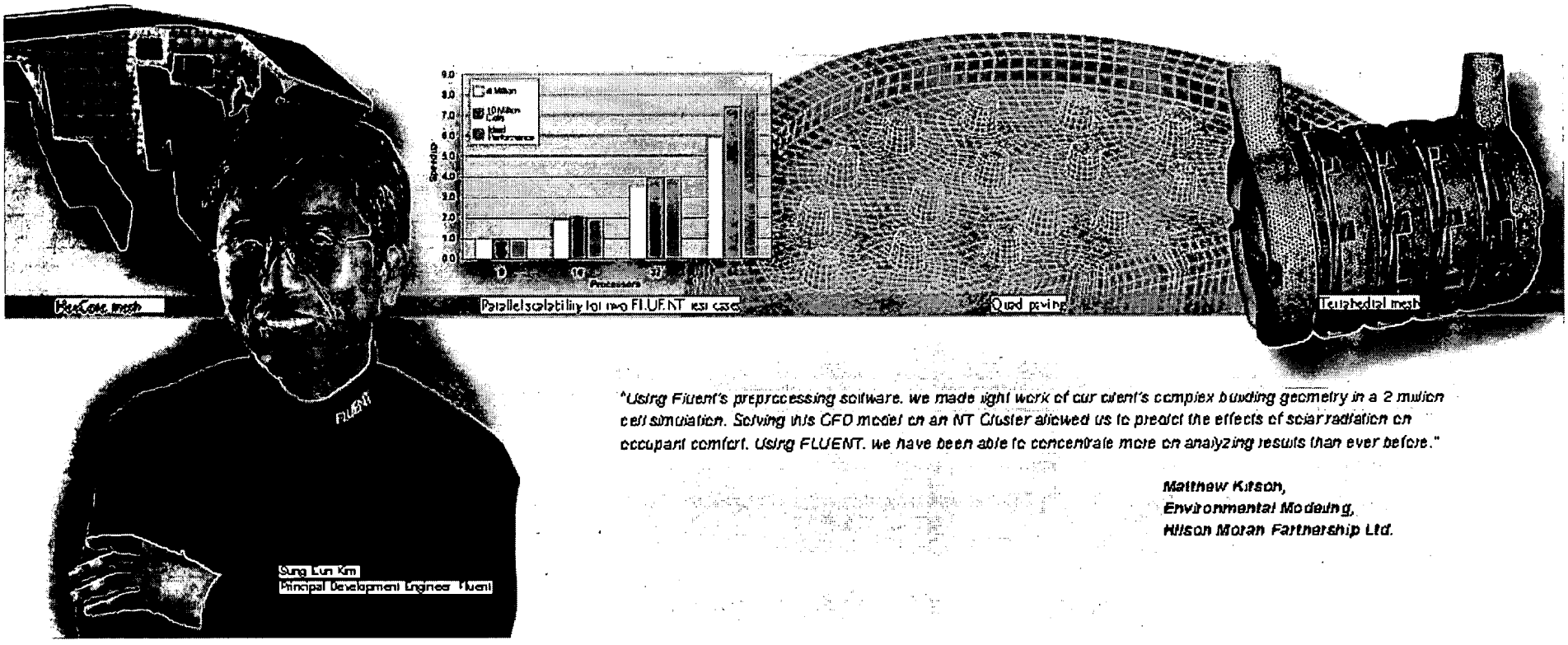
*"Fluent's CFD software has given us the ability to quickly predict the behavior of several design proposals that previously could not be modeled. We are also able to reduce our test time and expense by eliminating designs that do not perform as intended."*

***Raymond H. Horstman,***
***Environmental Control Systems,***
***Boeing Commercial Airplane Group***

# Grids, Numerics, Parallel Processing

At the core of any CFD calculation is a computational grid, used to divide the solution domain into thousands or millions of elements where the problem variables are computed and stored. In FLUENT, unstructured grid technology is used, which means that the grid can consist of elements in a variety of shapes: quadrilaterals and triangles for 2D simulations, and hexahedra, tetrahedra, prisms, and pyramids for 3D simulations. These elements, created using automated controls in GAMBIT, FLUENT's companion preprocessor, form an interlocking network throughout the volume where the fluid flow analysis takes place.

In the commercial CFD market today, no other provider offers more complex physical models on an unstructured grid than FLUENT. Sophisticated numerics and a robust solver ensure accurate results. The new non-iterative time advancement scheme has greatly reduced the time-to-solution for transient simulations. Mature parallel processing capabilities, available on NT, Linux, and Unix platforms, can be used on multiple processors of a single machine or multiple machines on a network. Dynamic load balancing automatically detects and analyzes parallel performance and adjusts the distribution of computational cells among the processors so that a balanced load is shared by the CPUs.



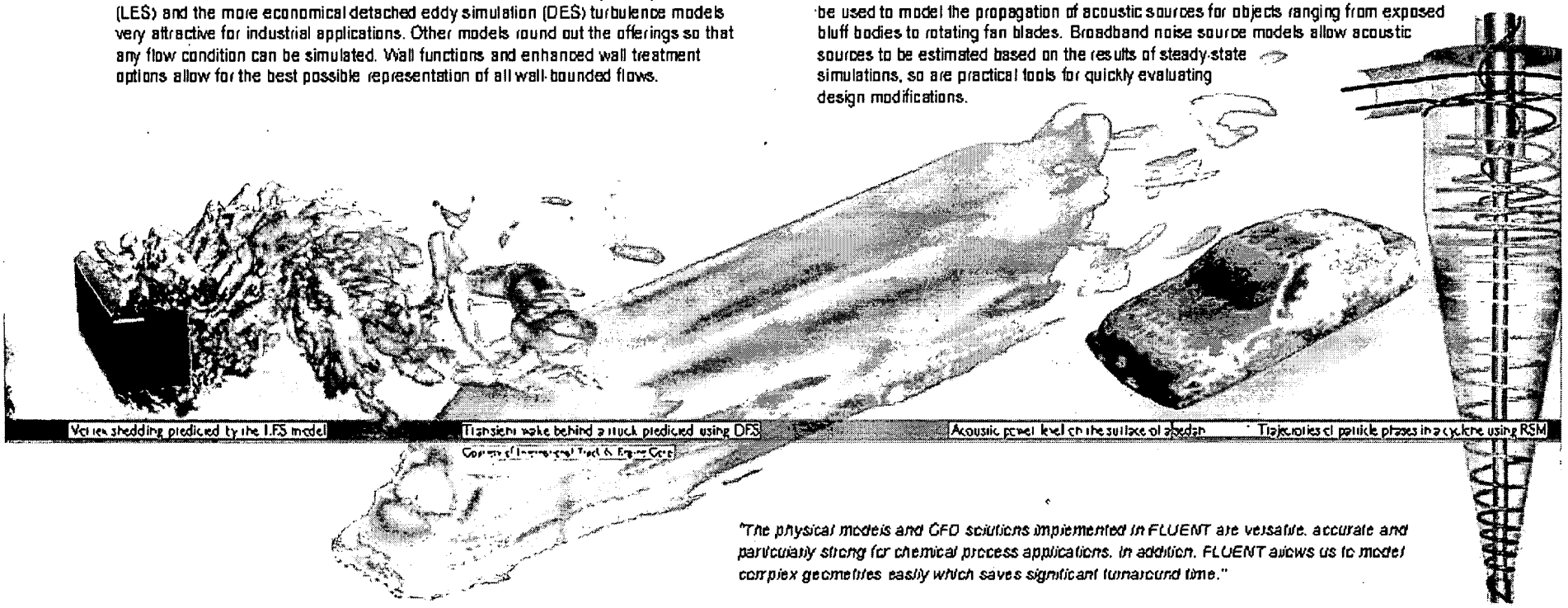

*"Using Fluent's preprocessing software, we made light work of our client's complex building geometry in a 2 million cell simulation. Solving this CFD model on an NT Cluster allowed us to predict the effects of solar radiation on occupant comfort. Using FLUENT, we have been able to concentrate more on analyzing results than ever before."*

***Matthew Kitson,***
***Environmental Modeling,***
***Hilson Moran Partnership Ltd.***

# Turbulence and Acoustics

FLUENT has always defined the cutting edge of turbulence modeling in commercial CFD software, offering an unparalleled breadth of models. Several versions of the heavily used and time-honored k-ε model are available, as is the Reynolds stress model (RSM) for highly swirling or anisotropic flows. Recent increases in computer power, coupled with decreases in cost, have combined to make large eddy simulation (LES) and the more economical detached eddy simulation (DES) turbulence models very attractive for industrial applications. Other models round out the offerings so that any flow condition can be simulated. Wall functions and enhanced wall treatment options allow for the best possible representation of all wall-bounded flows.

Aeroacoustics is an important focus for many industrial applications, but has traditionally been difficult to simulate. In FLUENT, the noise resulting from unsteady pressure fluctuations can now be computed in several ways. Transient LES predictions for surface pressure can be converted to a frequency spectrum using the built-in Fast Fourier Transform (FFT) tool. The Ffowcs-Williams & Hawkings acoustics analogy can be used to model the propagation of acoustic sources for objects ranging from exposed bluff bodies to rotating fan blades. Broadband noise source models allow acoustic sources to be estimated based on the results of steady-state simulations, so are practical tools for quickly evaluating design modifications.



Vortex shedding predicted by the LES model | Transient wake behind a truck predicted using DES | Acoustic power level on the surface of a loudspeaker | Trajectories of particle phases in a cyclone using RSM

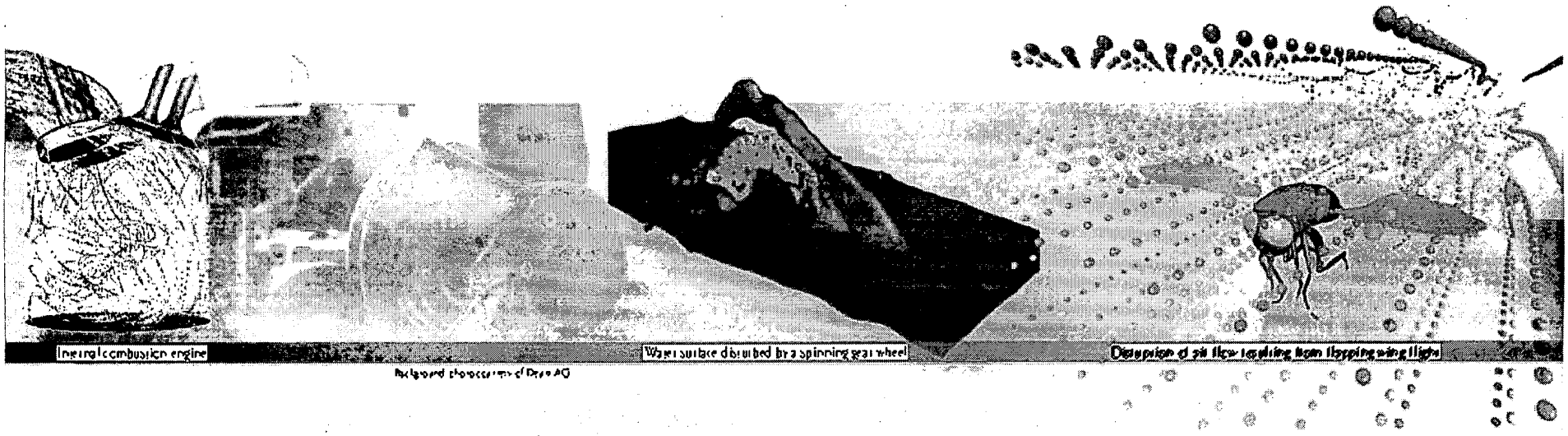
*"The physical models and CFD solutions implemented in FLUENT are versatile, accurate and particularly strong for chemical process applications. In addition, FLUENT allows us to model complex geometries easily which saves significant turnaround time."*

***Hiroaki Takehara,***
***Science and Technology Research Center,***
***Mitsubishi Chemical Corporation***

# Dynamic and Moving Mesh

Internal combustion engines, valves, store separation, and rocket launches are examples of problems where moving parts define the fluid flow. In FLUENT, the dynamic mesh capability meets the needs of these challenging applications. It has several different mesh rebuilding schemes, which can be used for different moving parts within the same simulation, as needed. Only the initial mesh and a description of the boundary movement are required. Dynamic meshing is compatible with a host of other models, including FLUENT's suite of spray breakup and combustion models, multiphase flow, free surface prediction, and compressible flow.

The periodic motion inside mixing tanks, pumps, and turbomachinery has traditionally been simulated with moving mesh models in FLUENT. The sliding mesh and multiple reference frames models have a proven track record and are fully compatible with other relevant models, such as LES, reacting, and multiphase flow.



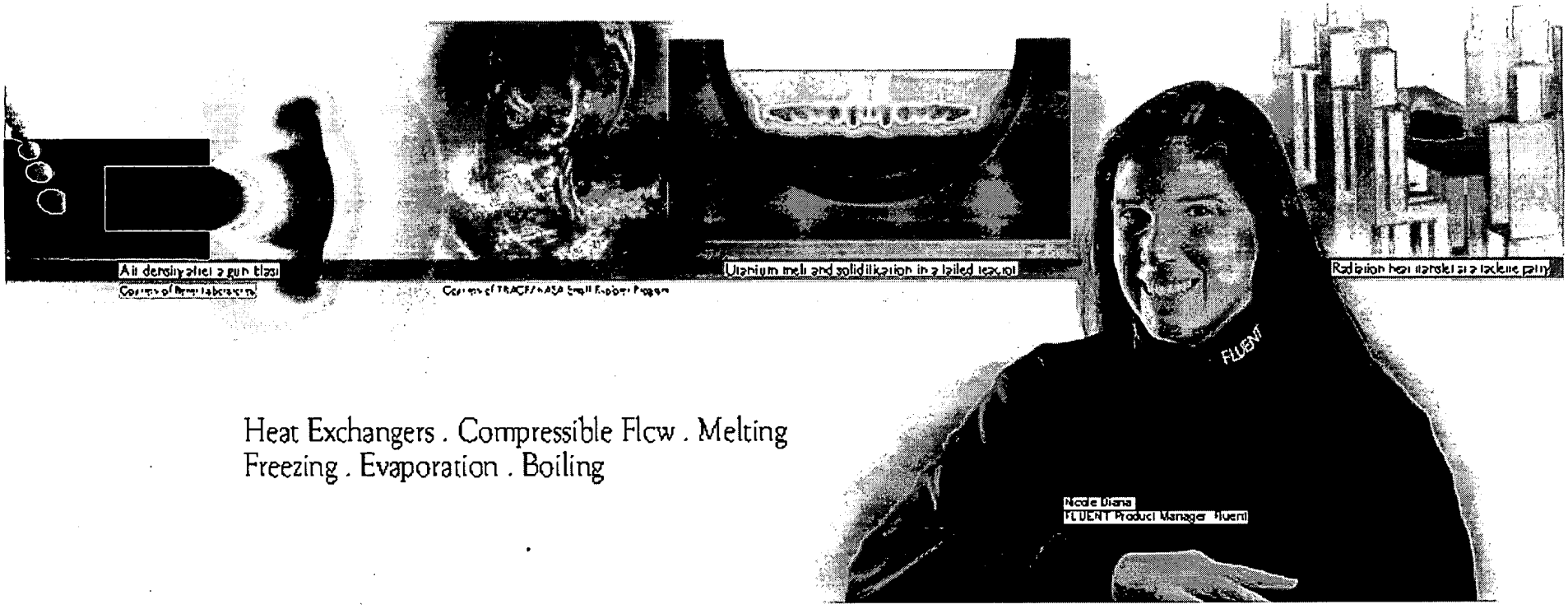

Background photograph of Daya AG

In-Cylinder . Store Separation . Passing Vehicles . Valves
Pumps . Turbomachinery . Mixing Tanks

# Heat Transfer, Phase Change, Radiation

Heat transfer accompanies many fluid flow phenomena and FLUENT offers a comprehensive suite of options for convection, conduction, and radiation. For radiation, the P1 and Rosseland models are available for environments with optically thick (participating) media, and a view-factor-based surface-to-surface model is available for environments with non-participating media. The discrete ordinates (DO) model is suited for any medium, including glass. A general-purpose discrete ray tracing model (DTRM) is also available. A solar load model makes use of a ray-tracing algorithm and includes a solar calculator. It allows for visualization of illuminated and shadowed areas, making climate control simulation results meaningful.

Other capabilities closely associated with heat transfer include models for cavitation, compressible liquids, heat exchangers, shell conduction, real gas, and wet steam. The phase change model tracks melting and freezing in the bulk fluid. Evaporation from droplets or wet particles and devolatilization from coal are available with the discrete phase model (DPM). The straightforward addition of heat sources and a complete set of thermal boundary condition options round out the capabilities, making heat transfer modeling in FLUENT a mature and reliable tool to meet any set of needs.



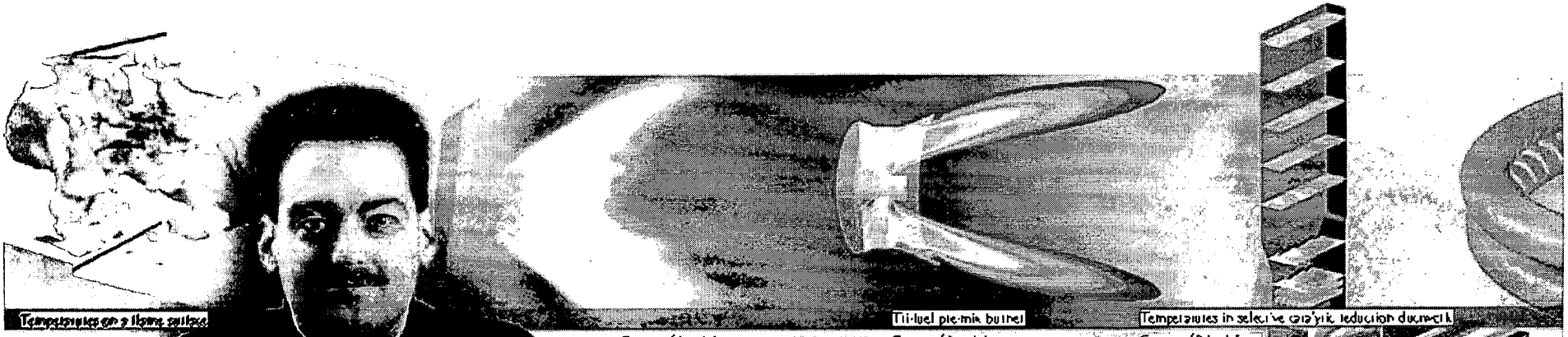

Heat Exchangers . Compressible Flow . Melting
Freezing . Evaporation . Boiling

# Reacting Flow

Chemical reaction modeling, especially in turbulent conditions, has been a hallmark of FLUENT software since its inception. Over the years, the comprehensive reaction modeling capabilities in FLUENT have helped engineers meet the diverse challenges of difficult combustion processes. The eddy dissipation concept, PDF transport, and stiff finite rate chemistry models have recently joined FLUENT's proven workhorses: the eddy dissipation, equilibrium mixture fraction, flamelet, and premixed combustion models for tackling a vast array of gaseous, coal, and liquid fuel combustion simulations. Models for the prediction of NOx formation are also widely used and customizable.

Many industrial applications involve reactions that take place on solid surfaces. FLUENT's surface reaction capability allows for reactions between gas and surface species as well as between different surface species, so that deposition and etching can be rigorously predicted. Simulations of catalytic converters, gas reformers, pollution control devices, and semiconductor manufacturing have all benefited from this technology.

FLUENT's reaction models can be used in conjunction with the LES and DES turbulence models. When these transient turbulence models are coupled with the reacting flow models, the power to predict flame stabilization and burnout becomes possible.



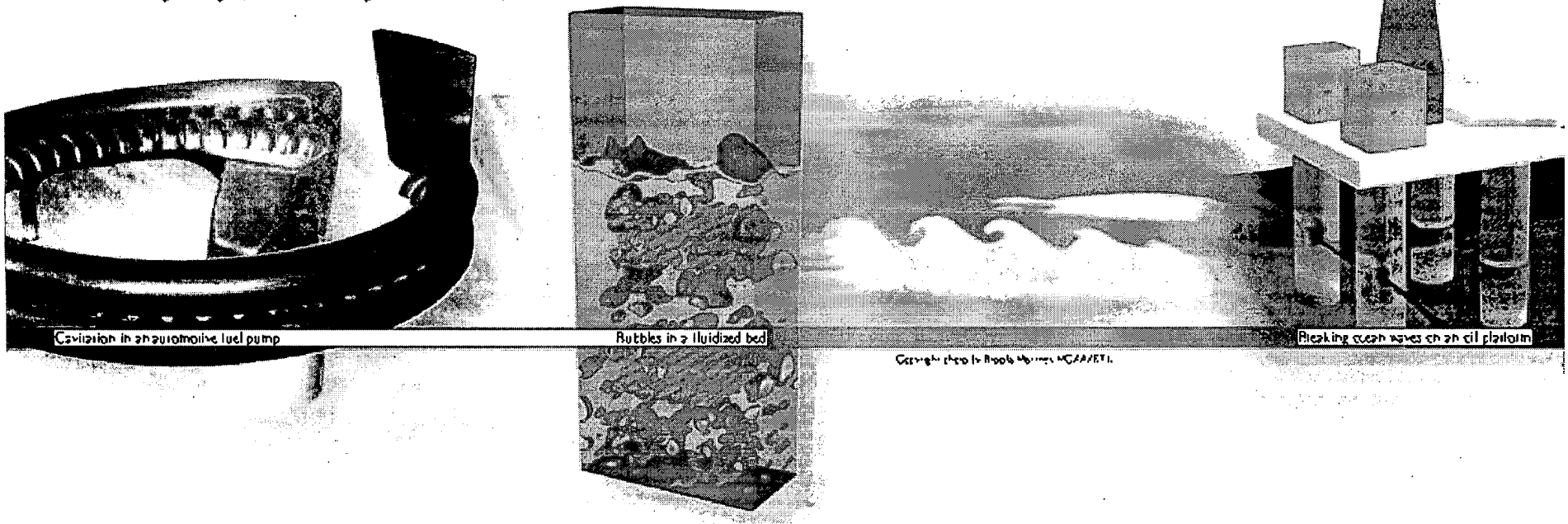


Gas Turbines . Boilers . Furnaces . Chemical Vapor Deposition
Erosion . Emissions . Flares . Etching . Catalytic Converters

# Multiphase

Multiphase mixtures are widespread in industrial applications, and FLUENT is a leader in multiphase modeling technology. Its varied capabilities allow engineers to gain insight into equipment that is often difficult to probe. The Eulerian multiphase model makes use of separate sets of fluid equations for interpenetrating fluids or phases. Special physics are available if one of the fluids is granular. In many cases, the more economical mixture model can be used for granular and non-granular mixtures as well. Three-phase mixtures (liquid, granular, and gas) can be modeled, so simulations of slurry bubble columns and trickle bed reactors are possible. Heat and mass transfer between phases can take place, making homogeneous and heterogeneous reactions possible.

Several other multiphase models are also standard in FLUENT. For some multiphase applications, such as spray dryers, coal furnaces, and liquid fuel sprays, the discrete phase model (DPM) can be used. Injections of particles, bubbles, or droplets can undergo heat, mass, and momentum transfer with the background fluid. The volume of fluid model is available for free surface flows, such as ocean waves, where the prediction of the interface is of interest. The cavitation model has proven useful for modeling hydrofoils, pumps, and fuel injectors. Boiling can be implemented though readily available user-defined functions.



Cavitation in an automotive fuel pump

Bubbles in a fluidized bed

Breaking ocean waves on an oil platform

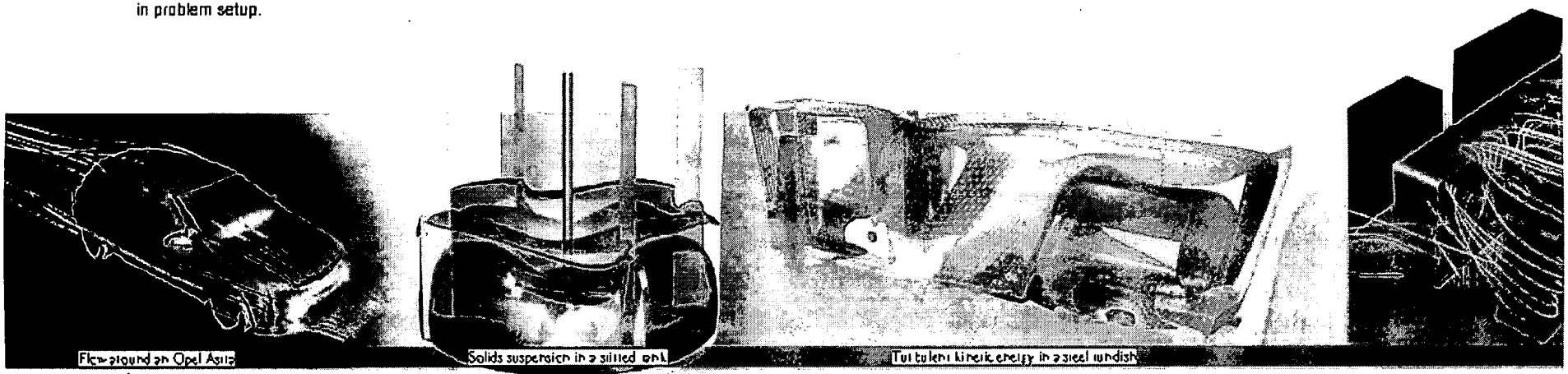


Bubble Columns . Fluidized Beds . Risers . Water Waves . Tank Sloshing . Separators
Spray Breakup . Cavitation . Boiling . Coal Burners . Spray Dryers

# Pre- and Postprocessing

Fluent offers software for the creation of problem geometries and grids. GAMBIT allows users to build geometries using basic construction tools. Alternatively, it can be used to read CAD files and condition the imported geometry for CFD analysis. For fast, flexible meshing, Fluent offers GAMBIT as well as TGrid, a state-of-the-art volume mesher. Both tools have many automated features for building or joining hybrid meshes with attention to boundary layers, nonuniform sizing, and core regions of hexahedral cells. For turbomachinery applications, GTurbo is available. This preprocessing tool uses familiar terminology and parametric templates to assist in problem setup.

FLUENT's postprocessing tools can be used to generate meaningful graphics, animations, and reports that make it easy to convey CFD results to engineers and non-engineers alike. Shaded and transparent surfaces, pathlines, and scene construction are just some of the postprocessing features that make FLUENT graphics unique. Solution data can be exported to third party graphics packages, or can be exported to CAE packages for additional analysis.



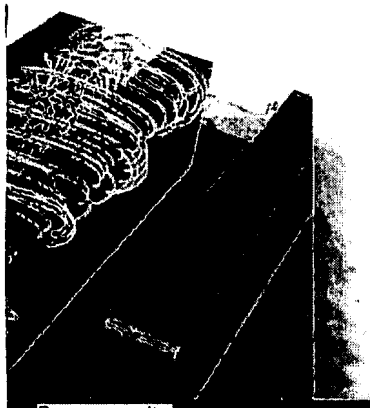

*"For a technology-based company like Norsk Hydro, CFD analysis using FLUENT has become an essential and accepted tool for problem analysis and optimization. FLUENT is used in all kinds of studies, from ventilation simulations via mixing analysis to complex multiphase separator calculations. We have come to appreciate the variety of models and the flexibility of the code. For us, FLUENT has proven to bring added value to the modeling process."*

***Eirik Manger,***
***Corporate Research Centre,***
***Norsk Hydro ASA***

# Customized Tools

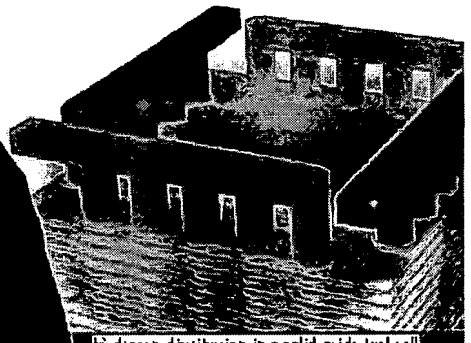
User-defined functions are a popular option for users wanting to customize FLUENT. Comprehensive documentation and a number of tutorials are available, as is full technical support. Fluent's global consulting network can provide or help create templates for the repeated setup of any type of equipment, such as cyclone separators, automotive HVAC systems, and furnaces. Add-on modules for many special applications are available, such as PEM and solid oxide fuel cells, magnetohydrodynamics, and continuous fiber drawing.

Fluent is proud to continue its long history of meeting customer needs across a breadth of industries and a myriad of applications. Clients receive technical support from some of the most knowledgeable flow modeling specialists in the business and can rely upon a wealth of core competencies as their needs dictate. Call your local office. See what FLUENT can do for your engineering process.



Gas cannel cooling

Pressure contours on a sizing and icing in a down-hole turbine



Hydrogen distribution in a solid oxide fuel cell

*"The FLUENT code is characterized above all by its user-friendliness and by its intuitive environment. Thanks to those features and its robust, accurate, and efficient solver, FLUENT has been readily adopted into our existing design process at the engine department. We now routinely use the code for simulation of engine related flows such as intake and exhaust systems."*

***Per Jonsson,***
***Scania CV AB***

Dipankar Choudhury
Chief Technology Officer Fluent

# Fluent Worldwide


**Corporate Headquarters**
Fluent Inc.
10 Cavendish Court
Lebanon, NH 03766, USA
Tel: 603 643 2600
Fax: 603 643 3967
Email: info@fluent.com

**US Regional Offices**
Ann Arbor, MI 48108
Tel: 734 213 6821

Austin, TX 78746
Tel: 512 306 9299

Evanston, IL 60201
Tel: 847 491 0200

Morgantown, WV 26505
Tel: 304 598 3770

Santa Clara, CA 95051
Tel: 408 522 8726

**European Regional Offices**
Fluent Benelux
Waver, Belgium
Tel: 32 10 45 12 61
Email: info@fluent.be

Fluent Deutschland GmbH
Darmstadt, Germany
Tel: 49 6151 36600
Email: info@fluent.de

Fluent Europe Ltd.
Sheffield, England
Tel: 44 114 281 8585
Email: info@fluent.co.uk

Fluent France SA
Montigny le Bretonneux, France
Tel: 33 1 3060 9897
Email: info@fluent.fr

Fluent Italia
Milano, Italy
Tel: 39 02 8901 3378
Email: info@fluent.it

Fluent Sweden AB
Göteborg, Sweden
Tel: 46 31 721 8780
Email: info@fluent.se

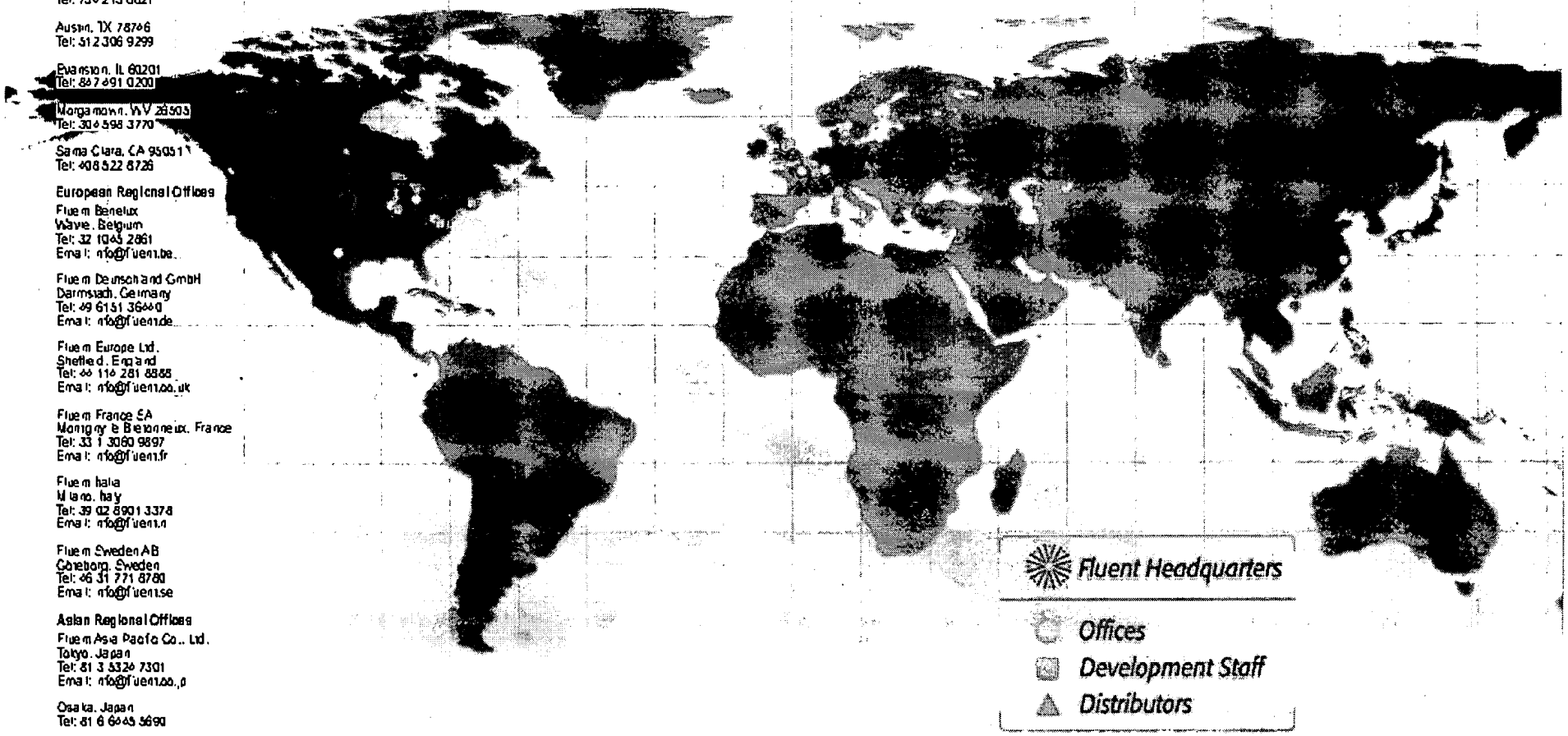
**Asian Regional Offices**
Fluent Asia Pacific Co., Ltd.
Tokyo, Japan
Tel: 81 3 5326 7301
Email: info@fluent.co.jp

Osaka, Japan
Tel: 81 6 6445 5690

Fluent China Holdings Ltd.
Shanghai, China
currently being established

Fluent India Pvt. Ltd.
Pune, India
Tel: 91 20 616 2500
Email: info@fluent.co.in

**Distributors**
For a full listing of our worldwide distributor network, go online to: www.fluent.com/worldwide/dist


LEBANON ANN ARBOR AUSTIN EVANSTON SANTA CLARA MORGANTOWN WAVRE DARMSTADT SHEFFIELD MONTIGNY LE BRETONNEUX
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